Chapter 4

Optical and photoelectrochemical properties of MoSe$_{2-x}$Te$_x$ ($x = 0.25, 0.5, 1, 1.5, 1.75$) single crystals

By “optical property” is meant a material’s response to exposure to electromagnetic radiation and in particular to visible light. When materials are exposed to electromagnetic radiation, it is sometimes important to be able to predict and alter their responses. This is possible when we are familiar with their optical properties and understand the mechanisms responsible for their optical behaviors. Knowledge of such properties of different materials can be used to design or improve any electrical or electronic device. The most widely used technique to understand the optical behaviour of any semiconductor material is the optical absorption spectroscopy. This chapter provides the results obtained by measurement of absorption spectra of 2H-MoSe$_{2-x}$Te$_x$ ($x = 0.25, 0.5, 1, 1.5, 1.75$) single crystals grown by chemical vapour transport technique.
4.1 INTRODUCTION

For device application of any semiconducting material, its optical properties play an important role. The optical band gap $E_g$, is the main optical parameter for semiconducting materials, while considering their use in a device application. Also energy gap of a semiconductor is the most crucial optical parameter which determines the efficiency of solar energy conversion. It has been shown [1] that for single crystals solar cells, $E_g$ should be around 1.3 eV for maximum solar energy conversion. The semiconductor materials having the band gap near to this optimum value are therefore considered as the most suitable for photovoltaic applications. It is, therefore, highly desirable that a determination of the optical band gap of the semiconducting material is a must. Energy band gaps are usually classified [2] in direct allowed, direct forbidden and indirect allowed, indirect forbidden gaps. Optical band gap of a material can be determined using the following methods.

1. Optical absorption
2. Photoelectrochemical methods
3. Intrinsic conduction measurements at high temperature
4. Photoemission
5. Band structure calculations

4.2 OPTICAL ANALYSIS

The most direct and the simplest method for probing the band structure of semiconductors are to measure the absorption spectrum. In the absorption process, a photon of a known energy excites an electron from lower to a higher-energy state. Thus by inserting a slab of semiconductor at the output of a monochromator and studying the changes in the transmitted radiation, one can discover all the possible transitions an electron can make and learn much about the distribution of states. Absorption is expressed in terms of coefficient $\alpha(h\nu)$, which is defined as
the relative rate of decrease in light intensity \( L(h\nu) \) along its propagation path:

\[
\alpha = \frac{1}{L(h\nu)} \frac{d[L(h\nu)]}{dx}
\]  

(4.1)

### 4.2.1 Fundamental absorption

Fundamental absorption refers to band-to-band transition, \( i.e. \), the excitation of an electron from valence band to conduction band. Fundamental absorption, which manifests itself by a rapid rise in absorption, can be used to determine the energy gap of a semiconductor. However, because the transitions are subjected to certain selection rules, estimation of an energy gap from the “absorption edge” is not a straightforward process—even if competing absorption process can be accounted for. Because the momentum of a photon, \( h/\lambda \), (\( \lambda \) is the wavelength of light and h is Planck’s constant), is very small compared to the crystal momentum \( h/\alpha \) (\( \alpha \) is the lattice constant), photon-absorption process should conserve the momentum of electron. Absorption coefficient \( \alpha h\nu \) for a given photon energy \( h\nu \) is proportional to the probability \( P_{if} \) for the transition from initial state, \( n_i \), and also to the density of available (empty) final state, \( n_f \), and this process must be assumed for all possible transitions between states separated by an energy difference equal to \( h\nu \):

\[
\alpha(h\nu) = A \sum P_{if} n_i n_f
\]  

(4.2)

Here, for simplicity we shall assume that all the lower states are filled and that all the upper states are empty, a condition which is true for undoped semiconductor at 0 K.

### 4.2.2 Direct and indirect band gap

The absorption process-taking place in a semiconductor can be described as an example of electronic transition processes, which are fully quantum mechanical in nature. These electronic transition processes give rise to
interband absorption in solids, which are of two types, known as direct and indirect transitions.

### 4.2.2.1 Direct band gap

Let us consider the transition between two direct valleys where all the momentum-conserving transition are allowed as shown in figure 4.1. Every initial state at $E_i$ is associated with a final state at $E_f$ such that

$$E_f = h\nu - |E_i|$$

(4.3)

But in parabolic bands,

$$E_f - E_g = \frac{\hbar^2 k^2}{2m_e^*}$$

(4.4)

and

$$E_i = \frac{\hbar^2 k^2}{2m_h^*}$$

(4.5)

Therefore,

$$h\nu - E_g = \frac{\hbar^2 k^2}{2} \left( \frac{1}{m_e^*} + \frac{1}{m_h^*} \right)$$

(4.6)

The density of directly associated states is

$$N(\nu)d(\nu) = \frac{8\pi k^2 dk}{(2k)}$$

(4.7)

$$N(\nu)d(\nu) = \frac{(2m_e^*)^{3/2}}{2\pi^2 \hbar^3} (h\nu - E_g)^{3/2} d(\nu)$$

(4.8)

Where $m_r$ is the reduced mass given by $\frac{1}{m_r^*} = \frac{1}{m_e^*} + \frac{1}{m_h^*}$. Hence the absorption coefficient is

$$\alpha(\nu) = A^* (h\nu - E_g)^{1/2}$$

(4.9)

Where $A^*$ is given as,
$A^* \approx q^2 \left( \frac{2m_p m_e^*}{m_h + m_e^*} \right)^{3/2}$

$q$ is the charge of electron

![Diagram showing direct transitions](image)

**Figure 4.1** Schematic diagram showing direct transitions.

### 4.2.2.2 Indirect transition between indirect valleys

When a transition requires a change in both energy and momentum, a double or two-step process is required because the photon cannot provide a change in momentum. Momentum is conserved via a phonon interaction, which is illustrated in figure 4.2. A quantum of lattice vibration, although a broad spectrum of phonon is available, only those with the required momentum changes are usable. These are usually the longitudinal and the transverse-acoustic phonons. Each of this phonon has a characteristic energy $E_p$. Hence to complete the transition $E_i$ to $E_f$ a phonon is either emitted or absorbed. These two processes are given respectively by

\[ h\nu_e = E_f - E_i + E_p \]  
\[ h\nu_b = E_f - E_i - E_p \]
Figure 4.2 Schematic diagram showing indirect transitions.

In general, however, at high temperature phonons are present and can participate in the absorption process. The optical transition is accordingly said to be non-vertical or indirect. Such indirect transitions are of great importance in semiconductors and provide a means of determining the energy band gap separating the top of the valence band and the bottom of the conduction band when these band extrema occur at different values of wave vector.

Optical absorption spectra of 2H-MoSe$_{2-x}$Te$_x$ (x = 0.25, 0.5, 1, 1.5, 1.75) single crystals were taken with the help of UV-VIS–NIR spectrophotometer in the wave length range of 200 nm - 3000 nm at room temperature. For
determination of band gap for semiconducting materials, absorption of incident photon by semiconducting material is an important technique. In this technique, photons of selected wavelengths are bombarded on the sample and their relative transmission is observed. Since the photons with energies greater than the band gap are absorbed while photons with energies less than band gap are transmitted, the technique provides accurate measurements of the energy band gap. The ratio of transmitted to incident radiation intensities is expected to depend on photon wavelength and the thickness of the sample.

When a photon beam of intensity \( I_0 \) (photons/(cm.sec)) transmits through a slab of a medium of thickness \( x \), the beam of photons attenuates in accordance with the exponential law

\[
I = I_0 e^{(-\alpha x)}
\]

Where \( \alpha \) is known as the absorption coefficient and it has unit of cm\(^{-1}\). This coefficient \( \alpha \) can be obtained simply by measuring \( I_0/I \) of the intensities impinging and emerging from the samples respectively.

### 4.2.3 Optical band gap determination

The relationship that exists for possible transitions across the energy gap of semiconductor, the absorption coefficient \( \alpha \) is proportional as follow [2],

\[
\alpha h\nu = A(h\nu - E_g)^\gamma
\]

for direct transitions and

\[
\alpha h\nu = \sum_j B_j (h\nu - E_g' \pm E_{py})^\gamma
\]

for indirect transitions.

Here, \( \alpha \) is the absorption coefficient, \( h\nu \) the energy of the incident photon, \( E_g \) the energy for the direct transition and \( E_g' \) the energy for indirect
transition and \( E_{pi} \) the energies of the phonons assisting at indirect transition. \( A \) and \( B \) are parameters depending in a more complicated way on temperature, photon energy and phonon energies \( E_p \).

However, for the analysis of the experimental results obtained at constant temperature, equations (4.14) and (4.15) are sufficient and they are most often used while interpreting results on absorption spectra obtained from semiconducting materials. The exponent ‘\( r \)’ in the above equations depends upon whether the transition is symmetry allowed or not and the constants \( A \) and \( B \) will assume different values for the allowed and forbidden transitions.

For indirect transitions the detailed form of equation (4.15) [3-5] is given as,

\[
\alpha_i = \sum_{i=1}^{1 \leq i \leq 2} \left\{ \frac{B_{ai}}{E} \left( \frac{1}{e^{\theta_i/T}}-1 \right) (E - E'_g + k\theta_i)^r + \frac{B_{ei}}{E} \left( \frac{1}{1-e^{\theta_i/T}} \right) (E - E'_g - k\theta_i)^r \right\} \tag{4.16}
\]

Where \( B_{ai} \) and \( B_{ei} \) are coefficients associated with absorption and emission of \( i^{th} \) phonon. \( E \) is the photon energy, \( E'_g \) the indirect energy gap and \( \theta_i \) is a phonon equivalent temperature defined by the equation,

\[
\theta_i = \frac{E_{pi}}{k} \tag{4.17}
\]

Where \( E_{pi} \) being the energy of \( i^{th} \) phonon.

In these cases the density of states is a constant independent of the energy and the expressions showing the dependence of \( \alpha \) in terms of direct and indirect transitions get modified [6] as

\[ \alpha = A'(h\nu - E_g)^\gamma \]  
\hspace{1cm} (4.18)

for direct transition and

\[ \alpha_i = \sum_{i=1}^{2} \left[ B_{ai}' \left( \frac{1}{e^{\theta_i/T} - 1} \right) (E - E'_{g} + k\theta)\gamma + B_{ei}' \left( \frac{1}{1 - e^{\theta_i/T}} \right) (E - E'_{g} - k\theta)\gamma \right] \]  
\hspace{1cm} (4.19)

for indirect transition [7].

### 4.3 EXPERIMENTAL

Samples were grown by chemical vapor transport technique. As grown samples exhibit n-type conductivity with electron concentration of $10^{15}$ to $10^{16}$ cm$^{-3}$ at room temperature. Thin samples for absorption measurement were obtained by cleavage. The optical absorption data were obtained by means of UV-VIS-NIR Spectrophotometer (Make: Perkin Elmer, Model: Lambda –19) shown in figure 4.3.

#### 4.3.1 UV-VIS-NIR Spectrophotometer

For obtaining the absorption spectra using UV-VIS-NIR spectrophotometer from single crystals specimens, thin flakes of as grown crystals are used. These flakes are pasted on a thick black paper with a cut exposing the crystal flake to the incident light. The reference used is a replica of the black paper, having the cut at exactly the same position as the crystal flake. This arrangement is necessary because the crystal size is smaller than that of the sample compartment. Blank glass slides can also be used as replica. All measurements were performed at room temperature with the incident beam normal to the basal plane of the grown crystal. Measurements parallel to basal plane could not be performed since the specimens were too thin to be mounted along this direction.
Figure 4.3 UV-VIS-NIR Spectrophotometer

Specifications

Facility: Double Beam, Double Monochromator, Ratio Recording

Lamp: Deuterium (UV), Tungsten-Halogen (VIS/NIR)

Detectors: Photomultiplier tube for UV-Visible, Lead-Sulphide cell (PbS) for NIR

Wavelength Range: 185-3200 nm

Scan speed: 0.3 to 1200 nm/min

Wavelength Accuracy: ±0.15 nm for UV/VIS & ±0.6 nm for NIR

Base line flatness: ± 0.001 Å, 4 nm slit

Ordinate Mode: Scan, Time Drive, Wavelength Programming, Concentration

Photometric Accuracy: ± 0.003 Å or ± 0.08 %T

Software used: PECOL Software for quantitative description of color
4.4 RESULTS AND DISCUSSION

The absorption spectra of $2\text{H-MoSe}_{2-x}\text{Te}_x$ ($x = 0.25, 0.5, 1, 1.5, 1.75$) single crystals over the spectrum range 200 nm to 3000 nm were taken. The absorption spectra of $2\text{H-MoSe}_{2-x}\text{Te}_x$ single crystals are shown in Figures 4.4 (a-e).

**Figure 4.4a** Optical absorption spectrum of $\text{MoSe}_{1.75}\text{Te}_{0.25}$ single crystal.

**Figure 4.4b** Optical absorption spectrum of $\text{MoSe}_{1.5}\text{Te}_{0.5}$ single crystal.
**Figure 4.4c** Optical absorption spectrum of MoSeTe single crystal.

**Figure 4.4d** Optical absorption spectrum of MoSe$_{0.5}$Te$_{1.5}$ single crystal.
**Figure 4.4e** Optical absorption spectrum of $\text{MoSe}_{0.25}\text{Te}_{1.75}$ single crystal.

Figures 4.4a-e show how absorbance varies with wavelength. The curve varies smoothly in the wavelength range above 1100-2400 nm for all the crystals. Extra features are observed for 2H-$\text{MoSe}_{1.75}\text{Te}_{0.25}$ single crystals which are classified in three regions. First is in the wavelength range of 330-415 nm, second is in the 760-890 nm and third is in the 2400-2800 nm. The interpretation of these different regions is as follow:

The small peak is observed in the range of 315-415 nm (figure 4.5a) which may corresponds to the local exciton involved in the optical absorption process. The sharp and intense absorption peak observed for 2H-$\text{MoSe}_{1.75}\text{Te}_{0.25}$ single crystal at 856 nm wave length (figure 4.4c) may due to the free carrier absorption involved in the process [10].
Figure 4.5a  The absorbance for $\lambda = 335-415$ nm.  

Figure 4.5b shows the electron intramolecular vibrational coupling. Two electrons are paired to give rise to centrosymmetric nature of the vibration. The energy of vibration and thus the wavelength of its absorption peak may be coupled with other vibrators in the molecule. A number of factors that extent of such coupling can be identified. Coupling requires that the vibrations be of the same symmetry class.

Figure 4.5c  The real and imaginary part of dielectric constant for $2H$-MoSe$_{1.75}$Te$_{0.25}$ single crystal.

Dispersion line shape in real part and imaginary part of dielectric constant (figure 4.5c) shows the peak at exactly at the same frequency or wavelength. These are called as Hanle curves. In these Hanle curves the real part of the dielectric constant is of the dispersion shape while the imaginary part is Lorentzian.
**Figure 4.6a** The variation of refractive index (n) and extinction co-efficient (k) with wavelength for 2H-MoSe$_{1.75}$Te$_{0.25}$ single crystal.

**Figure 4.6b** The variation of refractive index (n) and extinction co-efficient (k) with wavelength for 2H-MoSe$_{1.75}$Te$_{0.25}$ single crystal.
Figure 4.6c The variation of refractive index (n) and extinction co-efficient (k) with wavelength for 2H-MoSeTe single crystal.

Figure 4.6d The variation of refractive index (n) and extinction co-efficient (k) with wavelength for 2H-MoSe$_{0.5}$Te$_{1.5}$ single crystal.
Figure 4.6e The variation of refractive index (n) and extinction co-efficient (k) with wavelength for 2H-MoSe$_{0.25}$Te$_{1.75}$ single crystal.

Figures 4.6a-e shows the variation of refractive index (n) and extinction co-efficient with wavelength for 2H-MoSe$_{2-x}$Te$_{x}$ single crystals. Refractive index and extinction co-efficient are calculated from the standard relations. It shows remarkable instability between the wave length 860 to 1100 nm. The refractive index changes with the wave length may due to the interaction taking place between photons and electrons in 2H-MoSe$_{2-x}$Te$_{x}$ single crystals. This change in refractive index shows that the materials are absorbing light in this region.

In order to analyze the results from this spectrum in the vicinity of the absorption edge on the basis of two as well as three dimensional model, values of absorption coefficient $\alpha$ were determined at every interval of
1nm. Although MoX$_2$ (X = Se and Te) possesses indirect allowed transition, we have fitted only the functions for direct as well as indirect transitions ($\alpha$hv)$^2$ (cm$^{-1}$eV)$^2$ and ($\alpha$hv)$^{1/2}$ (cm$^{-1}$eV)$^{1/2}$ vs. hv (eV) respectively on the basis of three dimensional model. The interpretation of the experimental results viz. the dependence of absorption coefficient ‘$\alpha$’ in terms of direct as well as indirect transition can be performed with the help of formula 4.14 and using the various values of $r$ equal to 2 and $1/2$ respectively.

Accordingly, figures 4.7a-e show the spectral variations of ($\alpha$hv)$^2$ (cm$^{-1}$eV)$^2$ vs. hv (eV) and figures 4.7f-j show spectral variations of ($\alpha$hv)$^{1/2}$ (cm$^{-1}$eV)$^{1/2}$ vs. hv (eV) for 2H-MoSe$_{2-x}$Te$_x$ single crystals. Since the curves indicate continuous straight lines, it is quite possible that they may represent direct as well as indirect band to band transition. [3, 8-9].

![Graph](image-url)

**Figure 4.7a** Plot of ($\alpha$hv)$^2$ vs. hv for MoSe$_{1.75}$Te$_{0.25}$ single crystal.
Figure 4.7b Plot of $(\alpha h)^2$ vs. $h \nu$ for MoSe$_{1.5}$Te$_{0.5}$ single crystal.

Figure 4.7c Plot of $(\alpha h)^2$ vs. $h \nu$ for MoSeTe single crystal.
**Figure 4.7d** Plot of $(\alpha h \nu)^2$ vs. $h \nu$ for MoSe$_{0.5}$Te$_{1.5}$ single crystal.

**Figure 4.7e** Plot of $(\alpha h \nu)^2$ vs. $h \nu$ for MoSe$_{0.25}$Te$_{1.75}$ single crystal.
Figure 4.7f Plot of $(\alpha h v)^{1/2}$ vs. $h v$ for MoSe$_{1.75}$Te$_{0.25}$ single crystal.

Figure 4.7g Plot of $(\alpha h v)^{1/2}$ vs. $h v$ for MoSe$_{1.5}$Te$_{0.5}$ single crystal.
Figure 4.7h Plot of $(\alpha h v)^{1/2}$ vs. $h v$ for MoSeTe single crystal.

Figure 4.7i Plot of $(\alpha h v)^{1/2}$ vs. $h v$ for MoSe$_{0.5}$Te$_{1.5}$ single crystal.
Figure 4.7j Plot of $(a\nu)^{1/2}$ vs. $\nu$ for MoSe$_{0.25}$Te$_{1.75}$ single crystal.

Table 4.1 Values of direct and in direct band gap for 2H-MoSe$_{2-x}$Te$_x$ crystals.

<table>
<thead>
<tr>
<th>Crystal</th>
<th>Direct Band gap (eV)</th>
<th>Indirect Band gap (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2H-MoSe$<em>{1.75}$Te$</em>{0.25}$</td>
<td>1.27</td>
<td>1.17</td>
</tr>
<tr>
<td>2H-MoSe$<em>{1.5}$Te$</em>{0.5}$</td>
<td>1.25</td>
<td>1.14</td>
</tr>
<tr>
<td>2H-MoSeTe</td>
<td>1.23</td>
<td>1.09</td>
</tr>
<tr>
<td>2H-MoSe$<em>{0.5}$Te$</em>{1.5}$</td>
<td>1.21</td>
<td>1.02</td>
</tr>
<tr>
<td>2H-MoSe$<em>{0.25}$Te$</em>{1.75}$</td>
<td>1.19</td>
<td>0.93</td>
</tr>
</tbody>
</table>

From the Table 4.1 it can be seen that there is a great deal of agreement with indirect allowed type transitions and the values of the band gap for 2H-MoSe$_{2-x}$Te$_x$ lie between the values of band gap of MoSe$_2$ and MoTe$_2$ single crystals [10]. Although for 2H-MoSe$_{2-x}$Te$_x$ ($x = 0$ and 2), absorption near the fundamental edge due to the indirect allowed transition in the
process has been observed [10-11]. The observed indirect character of
band gap is a common property of hexagonal VIB-VIA compounds [12-13]
and it can be confirmed by band structure calculations [14-15].
It is interesting to note from table 4.1 that the optical band gap
determined from the spectral response of the crystals increases by
increasing selenium content in the 2H-MoSe$_{2-x}$Te$_x$. The atomic radius
decreases as we go from Te (1.37 Å) to Se (1.17Å) leading to changes in the
bond strengths and hence in the structure. Further the electro-negativity
of the atoms increases from Te (2.1) to Se (2.4) thereby indicating an
increase in the ionic nature of the bonding. As a result, an increase in the
resistivity and a decrease in the effective carrier concentration should be
expected which agree with the experimental observations.

4.5 PHOTOELECTROCHEMICAL SOLAR CELL
4.5.1 An introduction to basic principles of PEC solar cells
Mankind has regarded SUN as the biggest source of energy. Solar energy
coming down to the earth's surface per year is approximately ten
thousand times the worldwide energy consumption per year. Harnessing
solar energy has therefore, attracted the attention of the scientists,
technologists, economists, sociologists and politicians. Much effort has
therefore been directed towards developing new and better solar energy
conversion devices. A high degree of sophistication has been achieved in
the fabrication of p-n junction solar cells. However, a challenging problem
in solar energy research is solar energy storage. In 1970s an alternative
strategy was suggested in which a solid-liquid junction was used. In the
present work, use of solid-liquid junction has been made to take up the
strategy of direct conversion of solar energy into electricity. The
photoelectrochemical conversion of solar energy is attractive because
there is an opportunity of solar energy storage in the form of fuel, which is
easily transportable. Photoelectrochemical cell is generally referred as the
PEC cell.
A photoelectrochemical (PEC) solar cell is defined as a cell in which the irradiation by light of appropriate frequency of an electrode in contact with a suitable electrolyte produces a change in the electrode potential with respect to reference electrode (under open circuit conditions) or produces a change in the current flowing in the galvanic cell containing the electrode (under short circuit conditions) [16].

4.5.1.1 Photoconversion

Photons are the quanta of electromagnetic radiation. Traditionally, photoconversion is taken as a process through which the visible electromagnetic radiation is converted into electrical energy. In general, the photoconversion process involves interaction of these photons with materials, which give rise to

1. Photoemission from metallic surfaces and
2. Photoeffects in semiconductors.

Upon photo irradiation of semiconducting material and subsequent absorption of this radiation in the semiconductor, following processes may result

1. Excitation of electrons from valence band to the conduction band.
2. Excitation of electrons from and to the impurity atoms.
3. Excitation of electrons to higher energy states in the same band.
4. Excitation of excitonic states.
5. Excitation of phonons.

With one or more of the above kind of processes occurring, two kinds of photoeffects; namely - photoconductive and photovoltaic have generally been recognized. It may be pointed out that it is the photovoltaic effect, which is at the root of the liquid junction solar cells.

So far in all the previous chapters, the growth and characterizations of MoSe$_{2-x}$Te$_x$ has been discussed in detail. From all the above investigations
it is quite apparent that \( \text{MoSe}_2\text{Te}_x \) possesses the semiconducting behavior and indirect band gap around \( 0.9 \) – \( 1.2 \) eV. Generally, it is observed that the solar radiation reaching earth shows the maxima around \( 1.3 \) eV. Therefore if any device to be used has solar radiations as the input quantity, then the highest efficiency can be achieved provided the band gap of semiconductors lies near this maxima. In this context, it can be said from the optical characterizations of \( \text{MoSe}_2\text{Te}_x \) single crystals that these materials have an appropriate value of indirect band gap which lies close to the maxima of incident solar radiations. So the construction of a solar cells and its performance evaluation has been carried out for all these crystals. The twenty- first century has been predicted to be the "age of light," and, in anticipation of this, we have been interested in light-related chemical phenomena, that is, using light to induce chemical and electrochemical reactions. We have focused our main attention on reactions that might be useful for maintaining our environment, including hydrogen production, carbon dioxide reduction, and the destruction of pollutants. The total amount of solar energy impinging on the earth’s surface in one year is about \( 3 \times 10^{24} \) Joule, or approximately \( 10^4 \) times the worldwide yearly consumption of energy.

The search for the efficient conversion of solar energy into other useful forms is, in view of the increasing anxiety over the exhaustion of fossil energy resources and attendant global warming, one of the most important challenges for future research and technology development. In systems designed for the purpose of converting solar energy into electricity and/or chemicals, two principal criteria must be met. The first is absorption, by some chemical substance, of solar illumination, leading to the creation of electrons and holes. The second is the effective separation of these electron–hole pairs with little energetic loss, before they lose their input energy through recombination. Another well-known
example is the solar photovoltaic (PV) cell, in which the photo generated electron–hole pairs are driven efficiently in opposite directions by an electric field existing at the boundary between n- and p-type semiconductors or at that between a semiconductor and a metal (Schottky junction). A potential gradient can also be created at the interface between a semiconducting material and a liquid electrolyte. Hence, if a semiconductor is used as an electrode that is connected to another (counter) electrode, photo-excitation of the semiconductor can generate electrical work through an external load and simultaneously drive chemical (redox) reactions on the surfaces of each electrode. Similarly, when semiconductor particles are suspended in a liquid solution, excitation of the semiconductor can lead to redox processes in the interfacial region around each particle, but no electrical work is done, because the oxidation and reduction reactions are short-circuited. These types of systems have drawn the attention of a large number of investigators over the past twenty years, primarily in connection with the conversion of solar energy to electrical energy and chemically stored energy [17]. A survey of chalcogenides of the cheaply available materials suggests that among the low band gap semiconductors [18], little attention has been focused on chalcogenides of the sixth group metals molybdenum and tungsten [MX$_2$ where M = Mo or W and X = S, Se and Te] for their use in the conversion of solar energy to electrical energy or chemical energy via photoelectrochemical (PEC) cells. In all cases the electron hole separation and the electron transfer kinetics were found to be low, most probably due to the small size of the crystallites. To overcome these difficulties created by the presence of the grain boundaries which act as recombination centers, one should investigate the photoelectrochemistry of single crystals when they are available.
4.5.2. Primary Components of PEC Solar Cell

Photoelectrochemical cells are solar cells and extract electrical energy from light, including visible light. Each cell consists of a semiconducting photoanode and a metal cathode immersed in an electrolyte. A typical PEC has three primary components.

- Semiconductor electrode
- Counter electrode
- Electrolyte

4.5.2.1 Preparation of semiconductor electrode

A glass rod of 0.5 cm in diameter and 10 to 12 cm in length with a narrow bore of diameter 0.05 cm was used to prepare the electrode. One end of this narrow bore glass rod was flattened by hot gas blow. The flat portion was used as a platform for resting the crystal. The narrow bore was used as a passage for traversing a good conducting copper wire. The copper wire was flattened at one end for getting a contact with the crystal.

In the present work, a semiconductor electrode was fabricated in such a way that the contacting material (adhesive silver paste) provided good ohmic contact between the copper wire and the backside of the crystal. The whole assembly was then kept in an oven for few hours at 100°C for baking. After proper setting of the crystal on the copper wire terminal, the semiconductor was covered with an epoxy resin (araldite) leaving a light exposed an area of 2-5 mm² for exposure to light source. The so prepared complete device semiconductor electrode is shown in figure 4.8.
4.5.2.2 Counter electrode

A counter electrode in PEC solar cells is required to complete the electrochemical reactions in a cell for better performance of PEC solar cell. Generally platinum or graphite is widely used material for the same. Many materials have been investigated electrochemically as counter electrode materials, by Allen and Hickling [19]. Platinum is the standard counter electrode for PEC systems but its widespread use is impractical due to high cost and limited supplies. We can also use copper grid, tungsten carbide etc. In the present investigations, copper grid has been used in place of platinum as the counter electrode.

Figure 4.8 The semiconductor electrode.
4.5.2.3 Selection of appropriate electrolyte

The selection of electrolyte in a PEC solar cell is extremely important because it actually is a source for the electrochemical reactions leading to the photoeffects. The electrolyte consists of the oxidized and reduced species. These species should be ionic in nature, which help in transfer of photogenerated carriers from the photoelectrode to the counter electrode. To obtain a workable photoconversion from PEC solar cell, the selection of suitable electrolyte is very important. The electrolyte decides the band bending in the semiconductor near the interface and hence the efficiency of photoconversion. Among all electrolytes listed in table 4.2, it was observed that electrolyte with the composition 0.025M I₂ + 0.5M NaI + 0.5M Na₂SO₄ gave the minimum dark voltage ‘V_D’ and dark current ‘I_D’ and as well provided the maximum value of photocurrent (I_ph) and photovoltage (V_ph) for the electrodes which are used to fabricate PEC solar cell in present investigations. In this case, a mixture of iodine (I₂), sodium iodide (NaI) and sodium sulphate (Na₂SO₄) was employed as an electrolyte. All the chemical products were of reagent grade and the electrolyte solutions were prepared using triple distilled water. The solutions were not stirred during the measurement. Here photoelectrodes have been prepared using MoSe₂₋ₓTeX (x = 0.25, 0.5, 1, 1.5, 1.75) single crystals having visibly smooth surfaces.
Table 4.2 Lists of prepared electrolytes for present work.

<table>
<thead>
<tr>
<th>No.</th>
<th>Electrolyte Formula</th>
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<tbody>
<tr>
<td>1</td>
<td>0.025Ml₂ + 2MKI + 0.5MNa₂SO₄ +0.5MH₂SO₄</td>
</tr>
<tr>
<td>2</td>
<td>0.025Ml₂ + 2MKI + 0.5MNa₂SO₄</td>
</tr>
<tr>
<td>3</td>
<td>0.01Ml₂ + 2MKI + 0.5MNa₂SO₄</td>
</tr>
<tr>
<td>4</td>
<td>0.025Ml₂ + 2MKI</td>
</tr>
<tr>
<td>5</td>
<td>0.025Ml₂ + 1MKI + 0.5MNa₂SO₄ +0.5MH₂SO₄</td>
</tr>
<tr>
<td>6</td>
<td>0.025Ml₂ + 2MNaI + 0.5MNa₂SO₄</td>
</tr>
<tr>
<td>7</td>
<td>0.025Ml₂ + 0.5MNaI + 0.5MNa₂SO₄</td>
</tr>
<tr>
<td>8</td>
<td>0.025Ml₂ + 2MNaI + 2MNa₂SO₄ +0.5MH₂SO₄</td>
</tr>
<tr>
<td>9</td>
<td>0.025Ml₂ + 1MKI + 2MNa₂SO₄ +0.5MH₂SO₄</td>
</tr>
<tr>
<td>10</td>
<td>0.025Ml₂ + 1MNaI + 2MNa₂SO₄ +0.5MH₂SO₄</td>
</tr>
<tr>
<td>11</td>
<td>0.025Ml₂ + 2MNaI</td>
</tr>
<tr>
<td>12</td>
<td>0.1MK₄[Fe(CN)₆] + 0.1MK₃[Fe(CN)₆]</td>
</tr>
<tr>
<td>13</td>
<td>1MK₄[Fe(CN)₆] + 0.1MK₃[Fe(CN)₆]</td>
</tr>
<tr>
<td>14</td>
<td>0.1MK₄[Fe(CN)₆] + 1MK₃[Fe(CN)₆]</td>
</tr>
<tr>
<td>15</td>
<td>0.1MK₄[Fe(CN)₆] + 1MK₃[Fe(CN)₆]</td>
</tr>
<tr>
<td>16</td>
<td>0.1MFeCl₃ + 0.1MFeCl₂</td>
</tr>
<tr>
<td>17</td>
<td>0.05MFeCl₃ + 0.1MFeCl₂</td>
</tr>
<tr>
<td>18</td>
<td>0.01MFeCl₃ + 0.1MFeCl₂</td>
</tr>
<tr>
<td>19</td>
<td>1MFeCl₃ + 0.1MFeCl₂</td>
</tr>
</tbody>
</table>

4.5.3 Experimental Set up of Photoelectrochemical Solar Cell For V- I Characteristic

The semiconductor electrode prepared in the manner outlined above was immersed in an appropriate electrolyte contained in a corning glass beaker. A copper grid (3 cm x 3 cm) was used as the counter electrode. A schematic diagram of the photoelectrochemical solar cell is shown in figure 4.9a. The cell was illuminated with light from a Xenon lamp from
different intensities. The intensity of illumination was altered by changing the distance between the light source and the electrode.

Figure 4.9a The schematic diagram of PEC solar cell used to measure V-I characteristic.

The incident intensity of illumination was measured using ‘Suryampi’ or Solar meter (TES electrical electronic corporation TES 1332A). Photocurrent and photo-voltage were recorded using digital multimeters (Keithly Digital Multimeters) with accuracy of 0.1 mV/ µA. To vary the power point on the V- I characteristics, a series of variable resistance of different values has been used. In ideal cases and practical cases, the V-I characteristics of PEC solar cell is shown in figure 4.9b. Usually the V-I characteristics of practical cases deviate a lot from ideal characteristics.
4.5.4 Characteristic Parameters of PEC Solar Cells

There are various parameters available from which we can judge or evaluate the performance of PEC solar cell [20]. The most general parameters, which are used in everyday life for deciding the quality of the PEC solar cells, are efficiency, current and voltage specifications. Besides these, there are some other parameters which one must study in detail to improve the performance of such cells. The performance of a photovoltaic or PEC device can be described by the following measurements:

(a) the short circuit current
(b) the open circuit voltage
(c) the maximum power
(d) the fill factor
(e) the efficiency
(a) **Short circuit current** ($I_{sc}$)

The current measured directly across the electrodes in the absence of any load in the circuit is referred to as the short circuit current $I_{sc}$. Mathematically the short circuit current can be expressed as:

$$I_{sc} = I_0 \left[ \exp \left( \frac{eV_{oc}}{k_BT} \right) - 1 \right]$$  \hspace{1cm} (4.20)

where,

- $I_0$ = Reverse saturation current
- $k_B$ = Boltzmann constant
- $T$ = Operating temperature (Room temperature)
- $V_{oc}$ = Open circuit voltage

This parameter depends on the band gap of the semiconductor; smaller the band gap greater is the expected short circuit current.

(b) **Open circuit voltage** ($V_{oc}$)

The voltage measured across the electrodes when there is infinite load in the circuit is termed as the open circuit voltage $V_{oc}$. The mathematical representation of open circuit voltage is given below;

$$V_{oc} = \left( \frac{k_BT}{e} \right) \ln(I_L)$$  \hspace{1cm} (4.21)

where,

- $n$ is the ideality factor
- $k_B T / e = 0.0259$ volt (at 300K)
- $I_L$ = Intensity of illumination
(c) **Maximum power \( (P_m) \)**

The product of current and voltage gives the output power i.e.

\[
P_{\text{out}} = V \times I
\]

For a particular load resistance value, this output power will be maximum. This point is referred as the maximum power point and the value is called the maximum power \( (P_m) \).

(d) **Fill Factor (FF)**

Ideally a solar cell should have \( V_{mp} = V_x \) and \( I_{mp} = I_{sc} \) however, various loss mechanisms operating within the cell make it to deviate from the ideal behaviour. The term used to express this departure is known as the “fill factor” (FF) defined by

\[
F.F = \frac{J_{mp} \times V_{mp}}{J_{sc} \times V_{oc}}
\]

Where, \( J_{sc} \) is the short circuit current density

\( J_{mp} \) is the current density at maximum power point and

\( V_{mp} \) is the voltage at maximum power point.

(e) **Efficiency (\( \eta \))**

The theoretical conversion efficiency of a solar cell at the maximum power point is given by

\[
\eta = \frac{V_{mp} \times I_{mp}}{P_{in}} = \frac{F.F \times V_x \times I_{sc}}{P_{in}} \times 100\%
\]

Where \( P_{in} \) is the solar power input

\[
\eta = \frac{V_{mp} \times J_{mp}}{P_{in}}
\]

Where \( J_{mp} = I_{mp} / \text{Area} \)

The photo-electrode fabricated using \( \text{MoSe}_{2-x} \text{Te}_x \) (\( x = 0.25, 0.5, 1, 1.5, 1.75 \)) single crystals have been used as working semiconductor electrodes.
for the absorption of incident radiations. The electrolyte having concentration \([0.025 \text{M } \text{I}_2 + 0.5 \text{M } \text{NaI} + 0.5 \text{M } \text{Na}_2\text{SO}_4]\) have been used as the ionic conduction medium to support the charge transfer mechanism for PEC solar cells. Copper wire used as a counter electrode. The Xenon lamp has been used as a source of polychromatic light for the investigation of the photoconversion characteristic of \(\text{MoSe}_{2-x}\text{Te}_x\) \((x=0.25, 0.5, 1, 1.5, 1.75)\) based PEC solar cells.

**Figure 4.10a** Current Density \((J)\) vs. Photovoltage \((V_{ph})\) for \(\text{MoSe}_{1.75}\text{Te}_{0.25}\) crystal under different levels of illumination.
Figure 4.10b Current Density ($J$) vs. Photovoltage ($V_{ph}$) for $\text{MoSe}_{1.5}\text{Te}_{0.5}$ crystal under different levels of illumination.

Figure 4.10c Current Density ($J$) vs. Photovoltage ($V_{ph}$) for MoSeTe crystal under different levels of illumination.
Figure 4.10d Current Density ($J$) vs. Photovoltage ($V_{ph}$) for MoSe$_{0.5}$Te$_{1.5}$ crystal under different levels of illumination.

Figure 4.10e Current Density ($J$) vs. Photovoltage ($V_{ph}$) for MoSe$_{0.25}$Te$_{1.75}$ crystal under different levels of illumination.
Figures 4.10a-e depict that the photovoltage ($V_{ph}$) – photocurrent density ($J$) characteristics of the MoSe$_{2-x}$Te$_x$ ($x = 0.25, 0.5, 1, 1.5, 1.75$) electrodes obtained at various intensities in the range 10 mW/cm$^2$ – 90 mW/cm$^2$. It is quite apparent from figures 4.10a-e that the photovoltage characteristic deviates from the expected behavior for ideal solar cell. Also it can be said that the characteristics show the diverging behavior with increase in intensity. This is quite obvious because the increase in intensity of incident illumination directly means that the number of photons incident on the semiconducting materials surface also increases.

**Figure 4.11a** The variation of short circuit current ($I_{sc}$) with the intensity of incident illumination for MoSe$_{1.75}$Te$_{0.25}$ single crystal.
Figure 4.11b The variation of short circuit current ($I_{sc}$) with the intensity of incident illumination for MoSe$_{1.5}$Te$_{0.5}$ single crystal.

Figure 4.11c The variation of short circuit current ($I_{sc}$) with the intensity of incident illumination for MoSeTe single crystal.
Figure 4.11d The variation of short circuit current ($I_{sc}$) with the intensity of incident illumination for MoSe$_{0.5}$Te$_{1.5}$ single crystal.

Figure 4.11e The variation of short circuit current ($I_{sc}$) with the intensity of incident illumination for MoSe$_{0.25}$Te$_{1.75}$ single crystal.
Figures 4.11a-e show the variation of short circuit current with intensity of incident polychromatic illumination for all the grown samples. From these figures it is quite clear that the short circuit current increases with the intensity of incident illumination. But the important fact observed from figures 4.11a-e is that the increase is found to be nearly linear up to 90 mW/cm$^2$ intensity. This can be explained as under.

The absorption of incident radiations leads to the generation of electron-hole pairs within the semiconducting materials. It is always essential that the photo generated carriers within the semiconductor should take part in the charge transfer mechanism through the electrolyte and the counter electrode. This process can be divided in two steps.

- The efficient generation of carriers within the semiconductor due to the absorption of incident radiations.
- The oxidation-reduction which can also be called charge transfer reaction at semiconductor – electrolyte interface and the electrolyte – counter electrode interface.

If both the processes occur at the same rate, then the photocurrent always increases linearly with the increase in the intensity of incident radiations. But if the charge transfer mechanism across the two electrodes becomes slower than the photo generation mechanism, then there will not be a transfer of all generated photo carriers from semiconductor electrode to the counter electrode. This results into the nonlinear behavior of the characteristics which means that the short circuit current will start saturating after some intensity of light. The nonlinear behavior of $I_{sc}$ demonstrates that the recombination of generated photo carriers at the semiconductor electrolyte interface is limiting the rate of overall charge reactions over the higher values of light intensities employed.
Figure 4.12a The variation of open circuit voltage ($V_{oc}$) with the intensity of incident illumination for MoSe$_{1.75}$Te$_{0.25}$ single crystal.

Figure 4.12b The variation of open circuit voltage ($V_{oc}$) with the intensity of incident illumination for MoSe$_{1.5}$Te$_{0.5}$ single crystal.
Figure 4.12c The variation of open circuit voltage ($V_{oc}$) with the intensity of incident illumination for MoSeTe single crystal.

Figure 4.12d The variation of open circuit voltage ($V_{oc}$) with the intensity of incident illumination for MoSe$_{0.5}$Te$_{1.5}$ single crystal.
Figure 4.12e The variation of open circuit voltage ($V_{oc}$) with the intensity of incident illumination for MoSe$_{0.25}$Te$_{1.75}$ single crystal.

Similarly the open circuit voltages with intensity of incident radiations for all the electrodes have been shown in figures 4.12a-e. It is quite clear that variation of short circuit current and open circuit voltage with intensity of incident polychromatic illuminations is more or less of similar nature. This is quite expected.

The calculated parameters from the I-V characteristic are tabulated in table 4.3.
Table 4.3  Photoresponse of 2H-MoSe$_{2-x}$Te$_x$ single crystals as Photoelectrode.

<table>
<thead>
<tr>
<th>Electrolyte</th>
<th>0.025M I$_2$+ 0.5M NaI + 0.5M Na$_2$SO$_4$</th>
<th>Crystal</th>
<th>Parameters</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>2H-MoSe$<em>{1.75}$Te$</em>{0.25}$</td>
<td><strong>Intensity</strong></td>
<td>90 mW/cm$^2$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>I$_{sc}$</strong></td>
<td>10.3 µA</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>V$_{oc}$</strong></td>
<td>373 mV</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>P$_{max}$</strong></td>
<td>1360.3 x 10$^{-9}$ Watts</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>V$_{max}$</strong></td>
<td>218.0 mV</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>FF</strong></td>
<td>0.35</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>η (%)</strong></td>
<td>0.98</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>Area exposed</strong></td>
<td>5.47 x 10$^{-6}$ m$^2$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2H-MoSe$<em>{1.5}$Te$</em>{0.5}$</td>
<td><strong>Intensity</strong></td>
<td>90 mW/cm$^2$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>I$_{sc}$</strong></td>
<td>13.1 µA</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>V$_{oc}$</strong></td>
<td>398.2 mV</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>P$_{max}$</strong></td>
<td>1908.78 x 10$^{-9}$ Watts</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>V$_{max}$</strong></td>
<td>238.3 mV</td>
</tr>
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<td></td>
<td><strong>FF</strong></td>
<td>0.38</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>η (%)</strong></td>
<td>1.05</td>
</tr>
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<td></td>
<td></td>
<td></td>
<td><strong>Area exposed</strong></td>
<td>5.30 x 10$^{-6}$ m$^2$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2H-MoSeTe</td>
<td><strong>Intensity</strong></td>
<td>90 mW/cm$^2$</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td><strong>I$_{sc}$</strong></td>
<td>14.2 µA</td>
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<td></td>
<td></td>
<td></td>
<td><strong>V$_{oc}$</strong></td>
<td>402.6 mV</td>
</tr>
<tr>
<td>2H-MoSe&lt;sub&gt;0.5&lt;/sub&gt;Te&lt;sub&gt;1.5&lt;/sub&gt;</td>
<td>( P_{\text{max}} )</td>
<td>( 2360.3 \times 10^{-9} ) Watts</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-------------------------</td>
<td>----------------</td>
<td>---------------------------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( V_{\text{max}} )</td>
<td>246.2 mV</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>FF</td>
<td>0.46</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \eta (%) )</td>
<td>1.1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Area exposed</td>
<td>( 5.10 \times 10^{-6} ) m(^2)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>2H-MoSe&lt;sub&gt;0.25&lt;/sub&gt;Te&lt;sub&gt;1.75&lt;/sub&gt;</th>
<th>Intensity</th>
<th>90 mW/cm(^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>I(_{\text{sc}})</td>
<td>14.9 ( \mu )A</td>
<td></td>
</tr>
<tr>
<td>( V_{\text{oc}} )</td>
<td>408.3 mV</td>
<td></td>
</tr>
<tr>
<td>( P_{\text{max}} )</td>
<td>( 2789.6 \times 10^{-9} ) Watts</td>
<td></td>
</tr>
<tr>
<td>( V_{\text{max}} )</td>
<td>256.7 mV</td>
<td></td>
</tr>
<tr>
<td>FF</td>
<td>0.54</td>
<td></td>
</tr>
<tr>
<td>( \eta (%) )</td>
<td>1.17</td>
<td></td>
</tr>
<tr>
<td>Area exposed</td>
<td>( 5.10 \times 10^{-6} ) m(^2)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>2H-MoSe&lt;sub&gt;0.25&lt;/sub&gt;Te&lt;sub&gt;1.75&lt;/sub&gt;</th>
<th>Intensity</th>
<th>90 mW/cm(^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>I(_{\text{sc}})</td>
<td>15.3 ( \mu )A</td>
<td></td>
</tr>
<tr>
<td>( V_{\text{oc}} )</td>
<td>408.9 mV</td>
<td></td>
</tr>
<tr>
<td>( P_{\text{max}} )</td>
<td>( 3090.4 \times 10^{-9} ) Watts</td>
<td></td>
</tr>
<tr>
<td>( V_{\text{max}} )</td>
<td>260.3 mV</td>
<td></td>
</tr>
<tr>
<td>FF</td>
<td>0.59</td>
<td></td>
</tr>
<tr>
<td>( \eta (%) )</td>
<td>1.19</td>
<td></td>
</tr>
<tr>
<td>Area exposed</td>
<td>( 5.10 \times 10^{-6} ) m(^2)</td>
<td></td>
</tr>
</tbody>
</table>
The photoconversion efficiency and fill factor are also tabulated in table 4.3 for solar cell structure under different intensities of incident illuminations. In ideal case, I_{mp} = I_{sc} and V_{mp} = V_{oc}, but practically in the present case I_{mp} and V_{mp} deviate largely. As a result of this we have obtained lower fill factor. The overall conversion photo mechanism of PEC solar cell has so many factors [21-24].

4.6 CONCLUSIONS

It is now evident that the fundamental absorption edge in single crystal of 2H-MoSe_{2-x}Te_{x} is most probably due to the allowed indirect transition. It is seen that the three dimensional optical energy gaps of these materials vary from 0.93 eV to 1.17 eV at room temperature.

The material is found to be transparent for wavelengths above the fundamental edge. Moreover, the response remains constant up to the upper limit (2400 nm) of the measurement. Therefore, this material may be used for optical coating.

From the Photovoltage–Photocurrent characteristics of all the electrodes at various intensities it can be seen that photoconversion characteristic shows the diverging behavior with intensity and it deviates from the expected ideal behavior.

The short circuit current increases with intensity of illumination that is because of the fact that the charge transfer in those materials is due to the absorption of incident radiations and the oxidation-reduction processes at semiconductor – electrolyte interface and electrolyte – counter electrode interface. Open circuit voltage also shows the same.

From the obtained parameters of PEC it is concluded that the efficiency is increasing as the tellurium content in grown crystals increases. The maximum efficiency obtained for PEC solar cell is ~ 1.1%.
In this chapter, we have reported the optical properties of 2H-MoSe$_{2-x}$Te$_x$ through absorption spectroscopy. As we know that the physical properties of TMDCs are strongly affected by its layered structure. MoSe$_2$ and MoTe$_2$ are extensively studied for their electrical properties. Due to this reason, the subsequent chapters provide the pressure as well as temperature dependent electrical properties of 2H-MoSe$_{2-x}$Te$_x$ single crystals.
REFERENCES


